

A field function for the direct simulation of dense particulate flow with realistic multi-body collision modelling

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Abstract

In this paper, a novel field function is presented for low-memory-cost multimaterial mesh generation and fast collision detection. In addition, a multi-body collision model with parameterized elasticity and friction is devised for modelling deterministic and realistic particle-particle interactions. The devised field function and collision model are able to effectively achieve direct simulations of fluid-solid systems with dense and irregular particles.

1 Introduction

For the direct simulation of a fluid-solid system with dense and irregular particles, classifying the ownership of computational nodes and identifying numerical boundaries are prerequisites for numerical discretization implementation and interface condition enforcement, which problem can be referred to as multimaterial mesh generation.

For flows involving solid particles, interactions among the particles may exert a strong influence on the stresses in the fluid-solid mixture. Particle-particle collisions in a dense particle setting may even dominate the behavior of a multiphase system [1]. Therefore, collision modelling has a significant role in computing particulate flows.

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Modelling collisions in dense particle systems is undoubtedly complex and challenging. Comparing with experimentally correlated statistical models [1–3] and short-range repulsive force based collision [4, 5], interface-resolved collision modelling enables more accurate representation of the practical problems and enhances physical reality. However, additional challenges from collision detection and multi-body collision are introduced.

When surfaces of objects are explicitly represented by polygon meshes, collision detection by checking every object against every other object is very inefficient if the number of objects is large and the geometry of objects is complex. Considerable research has been devoted to optimizing the problem with strategies focusing on hierarchical object representation, orientation-based pruning criteria, spacial partitioning scheme, and distance computation algorithm [6–9]. One efficient approach for convex rigid body collision detection is a multi-level algorithm that integrates temporal coherence exploitation, pairwise pruning, and exact pairwise collision detection techniques to minimize collision detection operations for a dense particle system [7, 10].

Employing implicit surfaces defined by field functions has shown success in collision related modelling [8, 11, 12]. In the simulation of non-convex rigid body interactions, Guendelman et al. [8] advocates a dual geometry representation that an object is represented with both a Lagrangian triangulated surface and a signed distance function defined on an Eulerian grid. While triangulated surface representation allows accurate normal calculation and maintains sharp interfaces, using a signed distance function for each object enables convenient point inclusion test. For example, using the layer of grid points that is nearest to the zero isocontour of a signed distance function as sample points, the collision status can be determined by testing the values of the sample points with regard to other signed distance functions. Since surface resolution of implicitly defined surfaces is proportional to the grid resolution for field functions, good accuracy is able to be achieved when a well resolved grid is employed [8].

However, using signed distances as field functions for defining implicit surfaces consumes memory that is proportional to the number of represented particles. In addition, classifying the ownership of computational nodes and identifying numerical boundaries involve active fetching and comparing signed distances data scattered in the memory storage, which results in considerable cache missing when the number of particles is very large.

To solve multimaterial mesh generation on a Cartesian grid and to accelerate collision detection for a dense particle system, this paper proposes a novel integer field. For a computational domain embedded with a set of polyhedrons, the presented field function explicitly tracks all the polyhedron domains with multiple resolved interfacial node layers. As a result, this field function enables low-memory-cost multimaterial mesh generation and fast collision detection for computing particulate flows.

For resolving multi-body collision, a sequential pairwise collision approach is proposed in reference [8], in which pairwise collision sequentially repeats among interfering objects until all objects are separating at least once. Due to applying sequential collision, a temporal priority of the pairwise collisions is implicitly assumed. Although a random sampling of the collision queue can alleviate the temporal priority issue, deterministic modelling of the multi-body collision process is considered hard to achieve in this approach.

To achieve deterministic and realistic modelling of particle-particle interactions, this paper devises a multi-body collision model with parameterized elasticity and friction utilizing the idea of pairwise collision while completely removing the temporal priority among pairwise collisions. The effectiveness of the devised field function and collision model for the direct simulation of fluid-solid systems with dense and irregular particles are demonstrated through extensive numerical examples.

2 Method development

2.1 Field function description

Consider a spatial domain Ω discretized by a Cartesian grid $I \times J \times K$, and a set of polyhedron domains $\{\Omega_p : p = 1, \dots, P\}$ in space, introducing an additional domain Ω_0 as

$$\Omega_0 = \{x \in \Omega : x \notin \cup_{p=1}^P \Omega_p\} \quad (1)$$

To classify computational nodes inside Ω_m ($m = 0, \dots, P$) while identifying R layers of interfacial nodes, an integer type field function is introduced as

$$\Phi = \{(\phi, \varphi) : \phi \in \{0, \dots, P\}, \varphi \in \{0, \dots, R\}\} \quad (2)$$

where the domain identifier, ϕ , is determined by

$$\phi_{i,j,k} = m, \text{ if } x_{i,j,k} \in \Omega_m \quad (3)$$

And, the interfacial node layer identifier, φ , is determined by

$$\varphi_{i,j,k} = \begin{cases} r, & \text{if } \exists \phi_{i',j',k'} \neq \phi_{i,j,k} \text{ for } \begin{cases} |i' - i| = r, |j' - j| = 0, |k' - k| = 0 & \text{or} \\ |i' - i| = 0, |j' - j| = r, |k' - k| = 0 & \text{or} \\ |i' - i| = 0, |j' - j| = 0, |k' - k| = r & \text{or} \\ |i' - i| = r - 1, |j' - j| = r - 1, |k' - k| = 0 & \text{or} \\ |i' - i| = r - 1, |j' - j| = 0, |k' - k| = r - 1 & \text{or} \\ |i' - i| = 0, |j' - j| = r - 1, |k' - k| = r - 1 \end{cases} \\ 0, & \text{if } r > R \end{cases} \quad (4)$$

The criteria for domain identifier, ϕ , are based on the point inclusion results. The criteria for interfacial node layer identifier, φ , are based on the existence of a heterogeneous node on the discretization stencils of the tested node. Therefore, the determination of the value of φ depends on the type of differential operators presented in the governing equations as well as the type and order of the employed spatial discretization schemes.

To avoid either insufficient or excessive classification of interfacial nodes, the criteria in Eq. (4) may require to be adapted to the specific problem scenarios. For instance,

if no mixed derivatives are discretized, only line type stencils are involved in discretization. The conditional statements in Eq. (4) shall be reduced to

$$\begin{cases} |i' - i| = r, |j' - j| = 0, |k' - k| = 0 & \text{or} \\ |i' - i| = 0, |j' - j| = r, |k' - k| = 0 & \text{or} \\ |i' - i| = 0, |j' - j| = 0, |k' - k| = r \end{cases} \quad (5)$$

2.2 Multimaterial mesh generation

The field function $\Phi(\phi, \varphi)$ is able to generate a mesh utilized for computing multimaterial flows. As illustrated in Fig. 1, for a computational node (i, j, k) , $\phi_{i,j,k}$ gives the domain inclusion state of the node, and $\varphi_{i,j,k}$ contains the interfacial state of the node.

Let Ω_m be the solution domain, when the solution is conducted without using a ghost cell approach, $\Phi_{i,j,k}(\phi = m, \varphi = 0)$ describes a normal computational node while $\Phi_{i,j,k}(\phi = m, \varphi > 0)$ describes that the node (i, j, k) locates on the numerical boundaries. When a ghost-cell approach is employed, $\Phi_{i,j,k}(\phi = m, \varphi \geq 0)$ describes a normal computational node while $\Phi_{i,j,k}(\phi \neq m, \varphi > 0)$ with a neighbouring node $\Phi_{i',j',k'}(\phi = m, \varphi \geq 0)$ on the discretization stencils of the node (i, j, k) describes that the node (i, j, k) locates on the numerical boundaries of the computational domain Ω_m .

As a low-memory-cost integer field, the devised field function explicitly tracks all the problem domains with multiple resolved interfacial node layers. Therefore, employing this field function for a multimaterial problem, it is straightforward to enforce designated governing equations, constitutive models, numerical schemes, and interface conditions for each material domain.

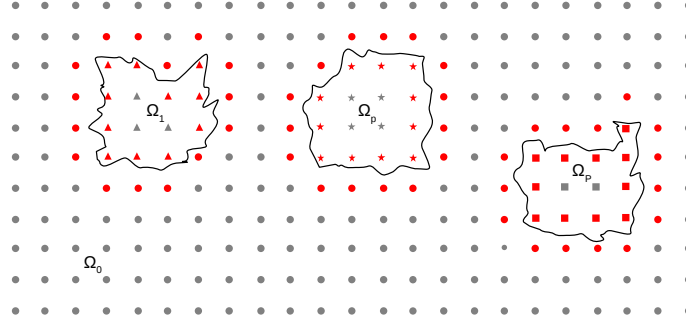


Figure 1: A 2D schematic diagram of the field function $\Phi(\phi, \varphi)$. Geometric shapes represent values of ϕ : circle, 0; triangle, 1; star, p ; square, P . Colors represent values of φ : grey, 0; red, 1; $R = 1$ is assumed here.

2.3 Collision detection

In addition to multimaterial mesh generation, the field function Φ also enables fast collision detection. As illustrated in Fig. 2, by sweeping through the nodes (i, j, k) with

$\Phi_{i,j,k}(\phi = p, \varphi = 1)$ for finding the neighbouring nodes (i', j', k') with $\Phi_{i',j',k'}(\phi \neq p, \varphi = 1)$, where $|i - i'| \leq 1$, $|j - j'| \leq 1$, and $|k - k'| \leq 1$, all the polyhedrons Ω_n colliding with the polyhedron Ω_p can be detected in an easy and efficient way.

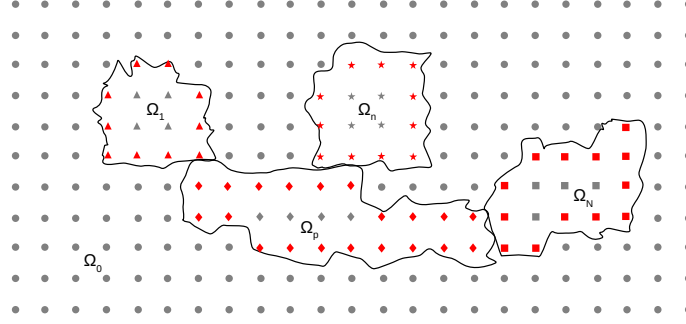


Figure 2: A 2D schematic diagram of applying the field function for collision detection. Geometric shapes represent values ϕ : circle, 0; triangle, 1; star, n ; square, N ; lozenge, p ; Colors represent values of φ : grey, 0; red, 1; $R = 1$ is assumed, and the interfacial nodes of Ω_0 are deactivated for the purpose of clarification.

When the polyhedron Ω_p collides with the polyhedron Ω_n , multiple elements such as vertices, edges, and faces on Ω_p may contact with multiple elements on Ω_n , in which one element on Ω_p may contact with either a portion of an element or multiple elements on Ω_n . This multi-contact problem introduces difficulties in the determination of the line of impact. Instead of finding the common normal of contacting geometric elements, an alternative approach is to approximate the line of impact via the Cartesian grid.

Suppose C computational nodes (i_c, j_c, k_c) in Ω_p satisfying $\Phi_{i_c,j_c,k_c}(\phi = p, \varphi = 1)$, and each (i_c, j_c, k_c) has D neighbouring nodes (i'_d, j'_d, k'_d) with $\Phi_{i'_d,j'_d,k'_d}(\phi = n, \varphi = 1)$, one possible approximation of the line of impact between Ω_p and Ω_n can be chosen as

$$\mathbf{e}_{pn} = \frac{\sum_{c=1}^C \sum_{d=1}^D [(i'_d - i_c)\mathbf{e}_1 + (j'_d - j_c)\mathbf{e}_2 + (k'_d - k_c)\mathbf{e}_3]}{|\sum_{c=1}^C \sum_{d=1}^D [(i'_d - i_c)\mathbf{e}_1 + (j'_d - j_c)\mathbf{e}_2 + (k'_d - k_c)\mathbf{e}_3]|} \quad (6)$$

where \mathbf{e}_1 , \mathbf{e}_2 , \mathbf{e}_3 are the unit direction vectors of the coordinate x , y , and z , respectively.

2.4 Multi-body collision

Suppose Ω_p collides with N polyhedrons Ω_n ($n = 1, \dots, N$). Denote the velocities of Ω_p as V_p and V'_p for before and after multi-body collision, respectively. Denote the velocities of Ω_n as V_n for before collision. To resolve multi-body collision while avoiding introducing temporal priority, pairwise collision (Ω_p, Ω_n) with the velocity state (V_p, V_n) is conducted to predict the post-collision velocity of Ω_p for the n -th pair collision:

$$V'_{p,n} = V_p - \frac{m_n}{m_p + m_n} (1 + C_R)(V_{pn} \cdot \mathbf{e}_{pn})\mathbf{e}_{pn} - C_f[V_{pn} - (V_{pn} \cdot \mathbf{e}_{pn})\mathbf{e}_{pn}] \quad (7)$$

where $V_{pn} = (V_p - V_n)$ is the relative velocity before collision, C_R is the coefficient of restitution in the normal direction ($C_R = 0$, $0 < C_R < 1$, and $C_R = 1$ are corresponding to perfectly inelastic collision, partially inelastic collision, and elastic collision, respectively), C_f is the coefficient of sliding friction, m_p and m_n are the mass of Ω_p and Ω_n , respectively.

Then a weighted post-collision velocity is adopted to approximate the final velocity of Ω_p :

$$V'_p = \frac{1}{N} \sum_{n=1}^N V'_{p,n} \quad (8)$$

After the above process is applied to each Ω_p ($p = 1, \dots, P$) in the particle system, a corresponding post multi-body collision velocity, V'_p , is obtained for each Ω_p . Then, the velocity state of the system is updated simultaneously.

2.5 Point inclusion test

To determine the value of ϕ requires classifying computational nodes of a Cartesian grid regarding a set of polyhedrons in space, which is a generalized point-in-polyhedron problem. For point inclusion test with regard to a single polyhedron, a variety of well-established methods, such as ray-crossing methods [13], angular methods [14], winding number methods [15], and signed distance methods [11], are available. The angle weighted pseudonormal signed distance computation method [16] provides good balance of efficiency and robustness. Meanwhile, it finds the closest point and the corresponding normal for a computational node, which is essential for implementing an immersed boundary method. In addition, the computed signed distance can be further employed for implementing a level-set method to track phase interfaces with topological changes.

3 Conclusion

To solve the multimaterial mesh generation on a Cartesian grid and to accelerate collision detection for a large multimaterial system, a novel integer field is devised. For a computational domain embedded with a set of polyhedrons, the presented field function explicitly tracks all the polyhedron domains with multiple resolved interfacial node layers. As a result, this field function enables low-memory-cost multimaterial mesh generation and fast collision detection for computing multimaterial flows. In addition, a multi-body collision model with parameterized elasticity and friction is devised for modelling deterministic and realistic particle-particle interactions. The devised field function and collision model are able to effectively achieve direct simulations of fluid-solid systems with dense and irregular particles.

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